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Adenine abundance in a collapsing molecular cloud

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Abstract : A vital ingredient of DNA molecule named adenine may be produced by successive addition of HCN during molecular cloud collapse and star formation. We compute its abundance in a collapsing cloud as a function of the reaction rate and show that in much of the circumstances, the resulting amount may be sufficient to contaminate planets, comets and meteorites We introduce a f-parameter which may be used to study the abundance where radiative association takes place.

Keywords : Molecular clouds, star formation, biomolecules.

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1. Introduction

In recent papers, Chakrabarti [1], and Chakrabarti and Chakrabarti ([2], hereafter referred to as Paper I) explored the possibility of the formation of biomolecules in star formation region using gas-phase chemistry. Their conclusion was that even in frigid condition in interstellar matter, some of the simplest amino acids such as glycine, alanine *etc.* could be produced even before the formation of stars and planets. Paper I also showed that with a choice of reaction rate constant 10^{-10}, significant adenine may also be produced. Some preliminary results of amino acids are in [1].

Adenine is a simply produced vital component of the DNA molecule and its significant production may point to an important clue into the problem of origin of life on planets like ours. Because of this, it is essential to carry out careful analysis on the reaction rates during the adenine formation. In Paper I, we used the formation of adenine by successive addition of HCN [3] by using an 'average' rate. In the normal circumstances, in gas-phase reaction HCN + HCN $\rightarrow$ $H_2C_2N_2$, rate would be small, since they must combine by radiative association, *i.e.*, they must radiate a photon when combined together.This is a slow process and the probability of photon emission could be 1 in a few thousand to a few million (T. Millar, private communication). However as the size of the molecule gets bigger, the process becomes faster. Thus, it is likely that for a large enough molecule, the radiative association may take place at every collision and at this stage, the collisional rate may be used. One possibility is therefore to assume that after every addition of HCN, the reaction rate goes up by a factor of f (f may be anywhere from 1 to 100 or more). Hence one may imagine that at the early stages, HCN + HCN $\rightarrow$ $H_2C_2N_2$ forms with a reaction rate of 10^{-16}, but for HCN + $H_2C_2N_2$, the rate becomes $f \times 10^{-16}$, for HCN + $H_3C_3N_3$, the rate becomes $f^2 \times 10^{-16}$ and so on. It would be therefore interest to learn, whether significant adenine is formed and it is detectable when the radiative association process is taken into account. In the present paper, we do just that. It is possible that more favorable reactions take place on ice, but in view of little known reaction rates of ice chemistry, we believe that the best we could do is to study the formation of these

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important molecules as a function of two parameters, namely, α_{Ad} and f. It is quite possible that a suitable f parameter we suggested above would take care of the ice-chemistry reaction rates as well. It is still possible that such an f may actually be determined by actual detection of molecules in space. Similarly, constancy of f is an assumption of our model. In reality it could vary with the size of the molecules.

So far, there has been controversy whether glycine has been observed in interstellar matter. Miao *et al* [4] tentatively detected glycine in the massive star forming region Sgr B2(N) though this was later challenged by Combes *et al* [5] who suggested that with the sensitivity of the detector taken into account, the lines were really at the confusion limit and positive identification would require more sensitive instruments. It is not known if any attempts were made to detect adenine lines, however there may have been detection of adenine in meteoritic samples (M. Bernstein, private communication).

2. Reaction network and hydrodynamic model

We choose the same reaction network as in Paper I which we again present here for the sake of completeness. We take the UMIST database (Millar, Farquhar & Willacy [6]) as our basis of chemical reactants and reactions, but added several new reactions such as synthesis of amino acids (alanine and glycine), hydroxyacids (glycolic and lactic acids), DNA base (adenine, [3]), urea synthesis *etc*. These new reactions make the total number of species to be 422. The rate coefficients of these additional reactions are difficult to find, especially in the environs of a molecular cloud. To use UMIST database, the rate constant for a two body reaction is written as [6],

$$k = \alpha(T/300)^{\beta}\exp(-\gamma/T)\ \mathrm{cm^3\,s^{-1}} \qquad (1)$$

where, α, β and γ are constants and T is the temperature. Amino acid synthesis rate was estimated from Figure 8 of Schulte and Shock [7]. Urea synthesis rate is kept comparable to the rates given in UMIST table. The rate constants were taken to be $\alpha = 10^{-10}$, $\beta = \gamma = 0$ for each two-body reactions. In Paper I, the rate constants for adenine synthesis was chosen to be similar to other two body reactions [$\alpha_{Ad} = 10^{-10}$, $\beta = \gamma = 0$ for each HCN addition in the chain HCN $\rightarrow$ (α_1) $\rightarrow$ CH(NH)CN $\rightarrow$ (α_2) $\rightarrow$ $NH_2CH(CN)_2$ $\rightarrow$ (α_3) $\rightarrow$ $NH_2(CN)C{=}C(CN)NH_2$ $\rightarrow$ (α_4) $\rightarrow$ $H_5C_5N_5$ (adenine)]. In the present paper, we run the same simulation with $\alpha_i|_{i=1,2,3,4} = \alpha_{Ad} = 10^{-12}$, 10^{-14}, 10^{-16} as well and in addition, consider the possibility that $\alpha_i = f^{i-1}\alpha_{Ad}$ as discussed in the introduction. In this notation, Paper I represents the case with $f = 1$.

Initial composition of the cloud before the simulation begins, is kept to be the same as in [6], and formation of H_2 is included using the grain-surface reaction with rates as in [6]. The initial *mass fractions* are taken to be the same as in [6] (but after appropriate convertion), *i.e.*, H : He : C : N : O : Na : Mg : Si : P : S : Cl : Fe = 0.64 : 0.35897 : 5.6×10^{-4} : 1.9×10^{-4} : 1.81×10^{-3} : 2.96×10^{-8} : 4.63×10^{-8} : 5.4×10^{-8} : 5.79×10^{-8} : 4.12×10^{-7} : 9×10^{-8} : 1.08×10^{-8}.

The hydrodynamic model is kept same as that in Paper I. We choose the initial size of the molecular cloud to be $r_0 = 3 \times 10^{18}$ cm, average temperature of the cloud $T =$ 10 K, and angular velocity of the cloud $\Omega = 10^{-16}$ rad s^{-1}. In this case, the speed of sound is $a_s \sim 19200$ cm s^{-1} and corresponding initial density [8] is $\rho = 10^{-22}$ g cm^{-3} and accretion rate is $\dot{M} = 1.06 \times 10^{20}$ g s^{-1}. In the isothermal phase of the cloud collapse, density $\rho \propto r^{-2}$ [9] and the velocity is constant. When opacity becomes high enough to trap radiations (say, at $r = r_{tr}$), the cloud collapses adiabatically with $\rho \propto r^{-3/2}$. In presence of rotation, centrifugal barrier forms at $r = r_c$, where centrifugal force balances gravity. Density falls off as $\rho \propto r^{-1/2}$ in this region [10]. The initial constant velocity of infall becomes 8900 cm s^{-1} and below $r = r_c$ velocity $\propto r^{-1/2}$ was chosen to preserve the accretion rate in a disk like structure of constant height. Since for the parameters chosen (generic as they are) $r_c > r_{tr}$, we chose $T \propto 1/r$ inside the centrifugal barrier ($r < r_c$) as in an adiabatic flow. We follow the collapse till a radius of 10^{12} cm is reached.

3. Models and results

We use the following models parameterized by α_{Ad} and f.

Model A : $\alpha_{Ad} = 10^{-16}$ and $f = 1$.
Model B : $\alpha_{Ad} = 10^{-14}$ and $f = 1$.
Model C : $\alpha_{Ad} = 10^{-12}$ and $f = 1$.
Model D : $\alpha_{Ad} = 10^{-10}$ and $f = 1$ (same as in Paper I).
Model E : $\alpha_{Ad} = 10^{-16}$ and $f = 100$.
Model F : $\alpha_{Ad} = 10^{-14}$ and $f = 10$.
Model G : $\alpha_{Ad} = 10^{-12}$ and $f = 5$.

Figure 1 shows the evolution of adenine abundance X_{Ad} with time (upper axis in seconds) and with logarithmic

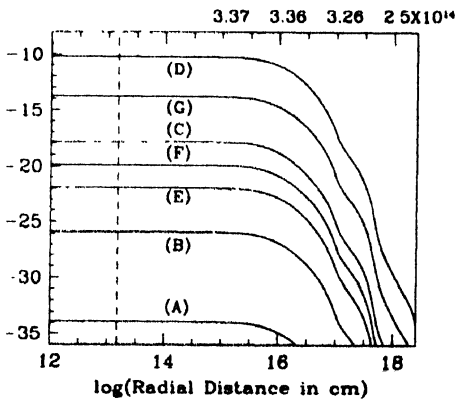

Figure 1. Evolution of adenine abundance with radial distance and time (upper axis) in a $\alpha - f$ model. Various models are marked on the curve See text for details.

radial distance (in cm). We note that generally speaking, at $r \sim 10^{16}$ cm, already the abundance X_{Ad} has reached almost the saturated value. This is because, as the upper axis indicates, most of the time is spent in this region during collapse. The final abundance in different models are : (A) $X_{Ad} = 1.36 \times 10^{-34}$, (B) 1.36×10^{-26}, (C) 1.36×10^{-18}, (D) 6.35×10^{-11}, (E) 1.2×10^{-22}, (F) 1.34×10^{-20} and (G) 1.8×10^{-14} respectively. Note that when X_{Ad} is really small, it is proportional to α_{Ad}^4 (for fixed f) as expected from a reaction with four sequence (see, *e.g*, Models A, B, and C). But when its abundance it significant, HCN otherwise participating in other reactions also contribute significantly to adenine formation. Similarly, at low X_{Ad}, for $f \neq 1$, the final abundance is proportional to f^6 for the same value of α_{Ad}.

If the present detectability limit of abundance is around 10^{-11} [5], then it is clear that adenine processed in our method should not be detectable (except for Model D) even though it may be enough to contaminate and flourish in some planets as we suggest. With a molecular weight of 135 for adenine, one could imagine that an abundance of 10^{-21} or less should really be considered as insignificant as far as the contamination theory goes. In that case, Models A, B and E must be rejected. This would correspond to a lower limit of $<\alpha_{Ad}>$ as $\sim 10^{-13}$ (where we use $<>$ to indicate an average over the whole chain of reactions leading the adenine formation from HCN). On the other hand, even when $\alpha_1 \sim <\alpha_{Ad}>$, f could be large enough to have eventual significant production (Model F). Thus, our $\alpha - f$ model implies that one needs to study the reaction rate of not only HCN + HCN $\rightarrow H_2C_2N_2$, but also every stages of HCN addition in order to come a definitive conclusion in this regard.

4. Conclusion

In presence of radiative association, adenine abundance X_{Ad} in an interstellar cloud seems to be roughly proportional to $\alpha_{Ad}^4 f^6$ for small X_{Ad}. This means that the measurements of both α_{Ad} and f must be made very accurately. We studied the $\alpha - f$ parameter space and found that while some region could produce significant abundance, a smaller region produce detectable (with present day technology) amount, while the rest produces abundance insignificant enough to dismiss the contamination theory. One must wait for the technological advancements to improve laboratory experiments in extreme conditions and to improve the detectability limit in order to come to a firm conclusion.

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